

Are the Tonks regimes in the continuum and on the lattice truly equivalent?

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Motivated by recent experiments, we compare the Tonks (*i.e.* hard-core boson gas) regime achieved in an optical lattice with the Tonks regime of a one-dimensional Bose gas in the continuum. For the lattice gas, we compute the local (*i.e.* on-site) two-body correlations as a function of temperature and the filling of the lattice. It is found that this function saturates to a constant value with increasing temperature. Furthermore, the parameter that characterizes the long-distance correlations in the lattice Tonks regime is also obtained, showing that on the lattice the long-distance correlations enter the Tonks regime more rapidly than in the continuum.

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Strongly interacting gases of bosons in one dimension have been recently realized using optical lattices [1, 2, 3]. By loading a Bose-Einstein condensate into a deep two-dimensional optical lattice, an array of one-dimensional atomic systems (tubes) was created [3, 4]. Strong correlations amongst the bosons were subsequently induced by turning on a third lattice along the axis of the tubes, which further decreases the ratio of kinetic to interaction energy [1, 2]. These anisotropic optical lattices exhibit a rich phase diagram [1, 5]. In particular, by making the third lattice deeper and reducing the filling of the lattice below one particle per site, the Tonks regime, where the bosons effectively become hard-core and behave in many respects like fermions, was reached in the experiments reported in Ref. 2. Time of flight measurements of the momentum distribution showed good agreement with a fermionization approach which accounted for finite temperature, finite-size, and trap effects [2].

The achievement of the Tonks regime in an optical lattice raises a number of questions about the equivalence of this system with the continuum Tonks regime. Mathematically speaking, the two types of Tonks gases correspond to the strongly interacting limit of two physically different models. The lattice Tonks gas (LTG) is obtained from the Bose-Hubbard model ($m = 1, \dots, M_0$),

$$H_{\text{BH}} = -\frac{J}{2} \sum_m (b_{m+1}^\dagger b_m + \text{H.c.}) + \frac{U}{2} \sum_m (b_m^\dagger)^2 (b_m)^2 \quad (1)$$

in the regime where $\gamma_L \equiv U/J \gg 1$ [19] and the filling of the lattice $f_0 = N_0/M_0 < 1$ (N_0 being the number of atoms and M_0 the number of lattice sites). However, the continuum Tonks gas (CTG) regime is obtained from the Lieb-Liniger model [6],

$$H_{\text{LL}} = \int_0^L dx \frac{\hbar^2}{2M} |\partial_x \Psi(x)|^2 + \frac{g}{2} (\Psi^\dagger(x))^2 (\Psi(x))^2 \quad (2)$$

when the parameter $\gamma \equiv Mg/\hbar^2 \rho_0 \gg 1$ [6, 7]. The presence of the density $\rho_0 = N_0/L$ in this parameter is a distinct feature of the continuum model. It means that the CTG regime can be reached either by increasing the interaction coupling g or by decreasing the density, ρ_0 . By contrast, the LTG regime can be reached by increasing the ratio $\gamma_L = U/J$ at any value of the filling f_0 . For low temperatures and fillings (*i.e.* $f_0 \ll 1$) the two Tonks regimes coincide since the Lieb-

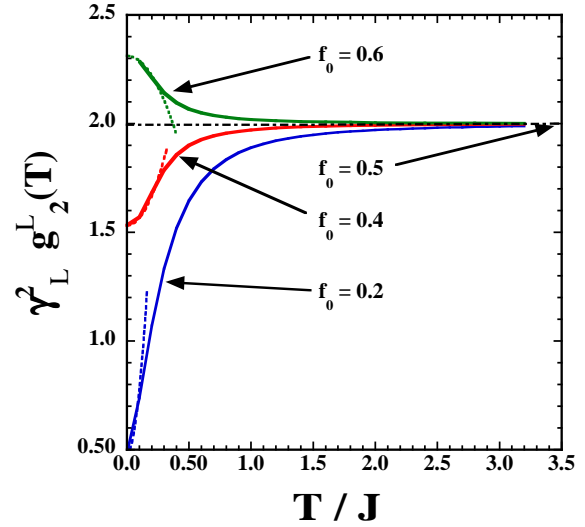


FIG. 1: Local two-body correlation function $g_2^L(T, f_0) = f_0^{-2} \langle (b_m^\dagger)^2 (b_m)^2 \rangle$ (times the square of $\gamma_L \equiv U/J \gg 1$) in the lattice Tonks regime, as a function of temperature T in units of the hopping J , for several lattice fillings $f_0 < 1$. At temperatures $T \gg J$, $g_2^L(T, f_0)$ saturates to the value at half-filling, which is temperature independent. This behavior should be contrasted with the monotonic increase at high temperatures of the corresponding function for the continuum (*i.e.* Lieb-Liniger) model: $g_2(T) = \rho_0^{-2} \langle (\Psi^\dagger(x))^2 (\Psi(x))^2 \rangle \propto T$ (see Refs. 8, 14). The dashed lines correspond to the low- T analytical approximation, Eq. (15).

Liniger model emerges as a low-density limit of the Bose-Hubbard model (see *e.g.* Ref. [8]). However, in [8] it was shown that, provided one has *at most* one particle per site (*i.e.* $n_m \leq 1$) and $U \gg J$, the Bose-Hubbard model can be effectively replaced by the following interacting fermion model:

$$H_F = -\frac{J}{2} \sum_m (c_{m+1}^\dagger c_m + \text{H.c.}) + H_1 + H_2, \quad (3)$$

$$H_1 = \frac{J}{2} \lambda_1 \sum_m (c_{m+1}^\dagger n_m c_{m-1} + \text{H.c.}), \quad (4)$$

$$H_2 = -J \lambda_2 \sum_m n_m n_{m+1}. \quad (5)$$

The couplings $\lambda_1 = \lambda_2 = \gamma_L^{-1} = J/U$ are small, and the fermions are ‘almost’ non-interacting. In this sense, therefore, one can speak of ‘fermionization’ of bosons. In this paper, we consider the regime where γ or γ_L are large, which should be of interest for current [1, 2, 3] and future experiments exploring these correlated systems.

The physical differences between the Tonks regimes of the Lieb-Liniger and Bose-Hubbard model can only be addressed by an explicit calculation of their correlation properties. These fall into two classes: short distance correlations are *non-universal* (i.e. model dependent), and therefore are expected to be different in the LTG and the CTG regimes. On the other hand, long-distance (or small momentum) correlations are characterized by the same power-laws *exactly* at the Tonks limit: γ or $\gamma_L \rightarrow +\infty$. Thus, for instance, in the thermodynamic limit at zero temperature, the momentum distribution $n(p) \sim p^{-1/2}$ for $p \ll \rho_0$ [9, 10]. Nevertheless, for finite values of γ or γ_L , long-distance correlations are characterized by the Luttinger-liquid parameter K (e.g. $n(p) \sim p^{1/2K-1}$), which is non-universal [12]. Precisely, these non-universal features in the two Tonks regimes are what interests us here. In this regard, it is important to notice that for the Bose-Hubbard model there is no exact (i.e. Bethe-ansatz) solution available [13], and therefore *analytical* results for non-universal properties are scarce. In what follows, we have summarized our results:

- In the LTG regime we have obtained the temperature and filling-fraction dependence of the on-site two-body correlation function $g_2^L(T, f_0) = f_0^{-2} \langle (b_m^\dagger)^2 (b_m)^2 \rangle$. This is the lattice counterpart of the continuum-model $g_2(T) = \rho_0^{-2} \langle (\Psi^\dagger(x))^2 (\Psi(x))^2 \rangle$. Both functions vanish for $\gamma, \gamma_L \rightarrow +\infty$, that is, when fermionization is complete. Whereas $g_2(T)$ was computed in Ref. [14] for all γ values, to the best of our knowledge no results existed for $g_2^L(T, f_0)$. For $\gamma_L \gg 1$ and temperatures $T \ll U$, we find:

$$g_2^L(T, f_0) = 2\gamma_L^{-2} \left(1 - \frac{f_2(T)}{f_0} \right) + O(\gamma_L^{-3}), \quad (6)$$

where $f_2(T) = \langle c_{m+2}^\dagger c_m \rangle$ (see below for details). At half-filling, the non-interacting fermion system is invariant under particle-hole symmetry: $c_m \rightarrow (-1)^m c_m^\dagger$, which implies that $f_2(T) = 0$ at all temperatures. Thus we obtain the result that $g_2^L(T, f_0 = 1/2) = 2\gamma_L^{-2}$, independent of T . Results for arbitrary temperatures and several fillings are shown in fig. 1. Although $g_2^L(T, f_0)$ is not directly related to the photo-association (PA) rate in the lattice because of the overlap between the Wannier orbitals at different sites, it should be experimentally accessible by suddenly ramping up the optical lattice before PA is performed in a time scale shorter than the atom tunneling time. After a substantial increase of lattice depth, overlap between the Wannier orbitals should become negligible.

- We have obtained the Luttinger-liquid parameters K and v_s for fillings $f_0 < 1$ to leading order in γ_L^{-1} :

$$K \simeq 1 + 4\gamma_L^{-1} \sin \pi f_0 / \pi, \quad (7)$$

$$v_s/v_F \simeq 1 - 4\gamma_L^{-1} (f_0 \cos \pi f_0). \quad (8)$$

where the Fermi velocity $v_F = Ja \sin \pi f_0 / \hbar$. Thus we conclude that the Tonks regime is more easily reached, as far as long distance correlations are concerned, on the lattice than in the continuum. To see this, consider for instance a half-filled lattice ($f_0 = 1/2$). Using the above formula for $\gamma_L = 10$, $K \simeq 1.13$, whereas for the Lieb-Liniger model [12] $K \simeq 1 + 4/\gamma = 1.4$ for $\gamma = \gamma_L = 10$ (Indeed, $\gamma = 10$ seems harder to achieve experimentally than $\gamma_L = 10$). The fact that long-distance correlations rapidly become Tonks-like for relatively shallow lattices justifies the fermionization treatment used in Ref. [2].

Next, we provide further details on the derivation of the above results. The key point is to notice that for temperatures $T \ll U$ and filling less than one particle per site, the Bose-Hubbard model, Eq. (1), can be effectively replaced by the fermionic model of Eq. (3), H_F . In particular, the replacement can be made for computing the (low-temperature) partition function of (1):

$$Z = \text{Tr} e^{-\beta(H_{\text{BH}} - \mu N)} = Z_0 \left\langle T e^{-\int_0^{\hbar\beta} \frac{d\sigma}{\hbar} H_{\text{int}}(\sigma)} \right\rangle, \quad (9)$$

where $\beta = 1/T$ and $H_{\text{int}} = H_1 + H_2$ (cf. Eqs. (4, 5)). In the second expression $Z_0 = \text{Tr} e^{-\beta(H_0 - \mu N)}$ and $\langle \dots \rangle = \text{Tr} [\rho_0(\mu, \beta) \dots]$, with $\rho_0(\mu, T) = e^{-\beta(H_0 - \mu N)} / Z_0$, and $H_0 = H_F - H_{\text{int}}$. We can now expand Z to the lowest order in γ_L^{-1} and obtain [20], $\log(Z/Z_0) = -\beta \langle H_{\text{int}} \rangle + O(\gamma_L^{-2})$. Thus we need to compute the thermal average of H_{int} , which can be readily done with the help of Wick’s theorem. The result can be written as follows:

$$\begin{aligned} \langle H_{\text{int}} \rangle = & \frac{1}{2} \lambda_1 J M_0 [f_0 (f_{+2} + f_{-2}) - (f_{+1}^2 + f_{-1}^2)] \\ & - \lambda_2 J M_0 [f_0^2 - f_{+1} f_{-1}] \end{aligned} \quad (10)$$

where we have denoted ($l = 0, \pm 1, \pm 2$):

$$f_l(T) = \langle c_{m+l}^\dagger c_m \rangle = \frac{1}{M_0} \sum_p e^{-i p l a} n(\epsilon_0(p), z), \quad (11)$$

the function $n(\epsilon, z) = [z^{-1} e^{\beta \epsilon} + 1]^{-1}$ is the Fermi-Dirac distribution for a fermion gas of fugacity $z \equiv e^{\beta \mu}$; $\epsilon_0(p) = -J \cos(pa)$ is the single-particle dispersion. Interestingly, all the above results follow from this simple expression, Eq. (10).

We begin by describing the calculation of $g_2^L(T, f_0)$. In an analogous manner to the continuum case [8, 14], this function can be obtained using the Hellmann-Feynman theorem:

$$g_2^L(T, f_0) = -\frac{2f_0^{-2}}{M_0\beta} \frac{\partial}{\partial U} \log Z \quad (12)$$

$$= 2f_0^{-2} \frac{\partial}{\partial U} \left(\frac{\langle H_{\text{int}} \rangle}{M_0} \right) + O(\gamma_L^{-3}). \quad (13)$$

By setting $\lambda_1 = \lambda_2 = \gamma_L^{-1}$ in (10), and assuming periodic boundary conditions [21] so that $f_l = f_{-l}$, one obtains the first result given above, Eq. (6). An alternative expression for $g_2^L(T, f_0)$ can be obtained after recasting

$$f_2(T) = f_0 \left(2J^{-2} \epsilon^2(T, z) - 1 \right), \quad (14)$$

where $\overline{\epsilon^2}(T, z) = f_0^{-1} \int d\epsilon \epsilon^2 g(\epsilon) n(\epsilon, z)$, being $g(\epsilon) = 1/\pi \sqrt{J^2 - \epsilon^2}$ the single-particle density of states. The advantage of this form of $f_2(T)$ is that the Sommerfeld expansion can be used to extract the low-temperature behavior:

$$g_2^L(T, f_0) = g_2^L(T=0, f_0) + \frac{4\pi}{3\gamma_L^2} \frac{(T/J)^2}{f_0 \tan \pi f_0} + O(\gamma_L^{-3}), \quad (15)$$

and $g_2^L(T=0, f_0) = 2\gamma_L^{-2} (1 - \sin(2\pi f_0)/2\pi f_0)$. It is worth noticing that in the low-filling limit $f_0 \rightarrow 0$ one recovers, from the above expression, the asymptotic expression for the Lieb-Liniger gas obtained in Ref. 14 (see also [8]), provided one makes the following identifications between the parameters of both models, $M \rightarrow \hbar^2/Ja^2$ (i.e. the effective mass), $g \rightarrow Ua$, $\rho_0 \rightarrow f_0/a$ (see [8]).

Finally, let us discuss some interesting properties of $f_0(T, z)$ and $f_2(T, z)$ defined in (11), and their implications for $g_2(T, f_0)$. The first property is a consequence of the particle-hole symmetry of the non-interacting spectrum, which implies that $f_0(T, z) + f_0(T, z^{-1}) = 1$, and hence that the fugacity for filling $1 - f_0$ is the inverse of the fugacity for filling f_0 . Likewise, one can show that $f_2(T, z) + f_2(T, z^{-1}) = 0$, which implies that in practice it suffices to compute $f_2(T, z)$ for fillings $f_0 \leq 1/2$. The other property of these functions explains the saturation of $g_2^L(T, f_0)$ with increasing temperature observed in fig. 1: for $T \gg J$, it can be shown that $z \rightarrow f_0/(1 - f_0)$ and $f_2(T, z) \rightarrow 0$; hence the local two-body correlation function $g_2(T, f_0) \rightarrow g_2(T, f_0 = 1/2)$ at all $f_0 < 1$. In the end, this is a consequence of the finite number of degrees of freedom available on the lattice.

We finally consider the non-universal aspects of long-distance correlations, which are parametrized by the Luttinger-liquid parameters K and v_s . In order to obtain the latter, it is convenient to work with the density and phase stiffness [12]:

$$v_J = \frac{\pi M_0 a}{\hbar} \frac{\partial^2 E_0(N_0)}{\partial \phi^2} \Big|_{\phi=0} \quad v_N = \frac{M_0 a}{\pi \hbar} \frac{\partial^2 E_0(\phi=0)}{\partial N^2} \Big|_{N_0} \quad (16)$$

The angle ϕ corresponds to a twist in the boundary conditions: $c_{m+M_0} = e^{i\phi} c_m$. This makes $f_{-l}(T=0) \neq f_l(T=0)$ for $l \neq 0$, and an explicit evaluation at finite size and zero temperature yields:

$$f_l(T=0, \phi) = \frac{e^{-i\phi l/M_0}}{M_0} \frac{\sin \pi l f_0}{\sin(\pi l/M_0)}. \quad (17)$$

Using that $K = \sqrt{v_J/v_N}$ and $v_s = \sqrt{v_N v_J}$ [12, 15] and, to leading order in γ_L^{-1} , $E_0 = \langle G|H_0|G \rangle + \langle G|H_{\text{int}}|G \rangle$, where $|G\rangle$ is the ground state of H_0 , along with (16), in the $M_0 \rightarrow \infty$ Eqs. (7) and (8) are obtained (the same expressions were also derived by carefully taking the field-theoretic continuum limit of H_F [18]).

Before concluding, an important difference between the Bose-Hubbard and Lieb-Liniger models is worth discussing: whereas the latter displays Galilean invariance, which implies that v_J must be equal to the Fermi velocity v_F [12], in the former this symmetry is broken by the lattice. By inspection of

Eq. (10) it can be seen that the terms responsible for the violation, that is, for the renormalization of v_J away from v_F are those those coming from H_1 . Thus, the renormalization of v_J becomes manifest after noticing that $[H_1, n_m] \neq 0$, and therefore one expects a non-zero contribution to the coefficient of $\partial_x j(x, t)$ ($j(x, t)$ being the long wave-length part of the current density) in the coarse-grained continuity equation [15]. This is one notable feature of H_F , which is obtained by projecting on a low-energy subspace where $n_m \leq 1$ [8], in what may be regarded as a first step of the renormalization group.

To sum up, we have shown that the Tonks regimes in the continuum and on the lattice are not, strictly speaking, equivalent. The local two-body correlations of the system on a lattice saturate with increasing temperature while for the Tonks regime of the continuum model are known to increase monotonically [8, 14]. Furthermore, the parameter K , characterizing the decay of long-distance correlations [12, 15], is more easily tuned to the Tonks limit on the lattice than in the continuum. Finally, our results can also be extended to the calculation of corrections to the internal energy and entropy of the lattice gas [18]. However, the distinct behavior of the two Tonks limits is well displayed by the properties considered in this work, and we shall not pursue this task here. This research has been supported through a *Gipuzkoa* fellowship granted by *Gipuzkoako Foru Aldundia* (Basque Country).

• **Appendix: On the equivalence of the first and second quantization approaches to fermionization.** The connection between fermionization in the wave function formalism and its second quantization version, which leads to effective Hamiltonians like Eq. (3), has not been sufficiently emphasized in previous treatments (e.g. Ref. 8). For completeness, we include a proof of their equivalence in this appendix.

In their pioneering 1928 paper on second quantization of fermion fields, Jordan and Wigner [16] introduced a transformation from hard-core bosons (or Pauli matrices) to fermions:

$$b_m = K_m c_m \quad b_m^\dagger = c_m^\dagger K_m, \quad (18)$$

$$K_m = \exp \left[i\pi \sum_{l < m} n_l \right] = \prod_{l < m} (1 - 2n_l). \quad (19)$$

The operator K_m (often referred to as the Jordan-Wigner string) turns the (hard-core) boson operator b_m into the fermionic c_m by attaching to it a phase factor which is determined by the number of particles to the left of site m . The trick converts the commutation relations of the b 's at different sites into the anti-commutation relations of the c 's. In this appendix, it is shown that the same trick yields the celebrated Bose-Fermi mapping due to Girardeau [17]. Let us consider the N -particle bra:

$$|\Phi\rangle = \sum_{\{m_i=1\}_{i=1}^{M_0}} \Phi_F(x_{m_1}, \dots, x_{m_N}) c_{m_1}^\dagger \cdots c_{m_N}^\dagger |0\rangle, \quad (20)$$

where $|0\rangle$ is the empty state. The wave function $\Phi_F(x_1, \dots, x_N)$ is anti-symmetric under exchange of any

pair of coordinates as a result of the anti-commutation of the c 's. This may lead us to think that the above bra describes a system of N fermions. However, by noticing that $K_m^{-1} = K_m$, we can invert (18) and write the product

$$c_{m_1}^\dagger \cdots c_{m_N}^\dagger |0\rangle = b_{m_1}^\dagger K_{m_1} \cdots b_{m_N}^\dagger K_{m_N} |0\rangle. \quad (21)$$

Next we shift all the string operators to the right and use that $K_m |0\rangle = |0\rangle$ (since $n_l |0\rangle = 0$ for all l) every time a string operator hits the empty state. Nevertheless, when commuting a string operator with a creation operator one must take care of a phase factor: $K_n b_m^\dagger = e^{i\pi\theta(x_n - x_m)} b_m^\dagger K_n$ (where $\theta(0) = 0$ is assumed). After shifting all the string operators to the right, a factor like this one appears for each pair of particles, and therefore,

$$c_{m_1}^\dagger \cdots c_{m_N}^\dagger |0\rangle = A(x_{m_1}, \dots, x_{m_N}) b_{m_1}^\dagger \cdots b_{m_N}^\dagger |0\rangle, \quad (22)$$

where the fully antisymmetric prefactor $A(x_{m_1}, \dots, x_{m_N}) =$

$e^{i\pi \sum_{i < j} \theta(x_{m_i} - x_{m_j})} = \prod_{i < j} \text{sgn}(x_{m_i} - x_{m_j})$. Introducing the last expression into (20), the bra can be rewritten as

$$|\Phi\rangle = \sum_{\{m_i=1\}_{i=1}^N}^{\{M_0\}} \Phi_B(x_{m_1}, \dots, x_{m_N}) b_{m_1}^\dagger \cdots b_{m_N}^\dagger |0\rangle, \quad (23)$$

where

$$\begin{aligned} \Phi_B(x_{m_1}, \dots, x_{m_N}) &= A(x_{m_1}, \dots, x_{m_N}) \Phi_F(x_{m_1}, \dots, x_{m_N}) \\ &= |\Phi_F(x_{m_1}, \dots, x_{m_N})| \end{aligned} \quad (24)$$

is a symmetric function which vanishes if $x_{m_i} = x_{m_j}$ for $i \neq j$. In other words, Φ_B is the wave function of a system of hard-core bosons. This proves the equivalence of the first and second quantization approaches to fermionization.

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 - [21] This requires N_0 to be odd, M_0 to be even and the ground state is non-degenerate.